Frameworks with crystallographic symmetry

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Abstract

Periodic frameworks with crystallographic symmetry are investigated from the perspective of a general deformation theory of periodic bar-and-joint structures in R^d. It is shown that natural parametrizations provide affine section descriptions for families of frameworks with a specified graph and symmetry. A simple geometric setting for diaplacive phase transitions is obtained. Upper bounds are derived for the number of realizations of minimally rigid periodic graphs.

Introduction

The notions of periodic graph and periodic framework emerged as abstractions of crystal structures. Inquiries about lattice sphere packings sprang from the same source.

We show that a classical perspective used in the theory of positive definite quadratic forms and lattice sphere packins leads to natural parametrizations for placements of periodic graphs. In this setting, all placements with a specified crystallographic symmetry correspond with a certain affine section. As a result, the deformation theory for periodic frameworks presented in our papers [BS2, BS3] is adapted in a natural way so as to encompass all cases of higher crystallographic symmetry.

1 Symmetries of a periodic framework

We adopt here definitions introduced in [BS2]. Let (G, Γ) be a d-periodic graph. The infinite graph $G = (V, E)$ is assumed connected and when given a periodic placement (p, π) in R^d, the corresponding periodic framework is denoted (G, Γ, p, π). Recall that $\Gamma \subset Aut(G)$ is a free Abelian group of rank d and π is a faithful representation of Γ by a lattice of translations of rank d. Moreover,

$$p : V \to R^d \quad \text{and} \quad \pi : \Gamma \to \mathcal{T}(R^d) \tag{1}$$

are related by:

$$p \circ \gamma = \pi(\gamma) \circ p \quad \text{for all } \gamma \in \Gamma \tag{2}$$

Relation (2) shows that π may be inferred from p, but most considerations about framework deformations and symmetries benefit from observing both functions. The quotient multigraph G/Γ is assumed to be finite and we put

$$n = |V/\Gamma| \quad \text{and} \quad m = |E/\Gamma| \tag{3}$$

Periodic frameworks are abstract, idealized versions of crystalline materials and, like them, may posess other symmetries, besides those expressing periodicity under Γ. Thus, there might be a larger group of automorphisms $\Gamma \subset \Sigma \subset Aut(G)$ and an extension of π to a faithful representation of Σ by a crystallographic group $\pi(\Sigma) \subset E(d)$, such that relation (2) would hold for all $\sigma \in \Sigma$.

Considering that $Aut(G, \Gamma)$ is the normalizer of Γ in $Aut(G)$, a natural assumption for investigating this setup will be that Γ is *normal* in Σ, that is $\Gamma \subset \Sigma \subset Aut(G, \Gamma)$. If all translational symmetries of the framework (G, Γ, p, π) are in $\pi(\Gamma)$, this is necessarily the case, since the subgroup of translations in a crystallographic group is normal. In general, the normality assumption would hold after replacing the initial periodicity group Γ by an appropriate subgroup of finite index $\tilde{\Gamma} \subset \Gamma$. Alternatively, instead of relaxing, one may refine the periodicity group by adopting all translational symmetries of the given framework.

For these reasons, we proceed below with the study of framework symmetries which correspond to graph automorphisms in the normalizer $N(\Gamma)$ of Γ in $Aut(G)$. Note that the quotient group $N(\Gamma)/\Gamma$ acts naturally on the quotient graph G/Γ. It follows that $N(\Gamma)/\Gamma$ is finite, since G/Γ is finite and G connected.

Definition 1 *We say that $\sigma \in N(\Gamma) = Aut(G, \Gamma)$ is a symmetry of the d-periodic framework (G, Γ, p, π) when the result of acting by σ on the framework is the same as the result of acting by an isometry $s \in E(d)$, that is:*

$$s \circ p = p \circ \sigma \tag{4}$$

In other words, we have a commutative diagram

$$\begin{array}{ccc} V & \xrightarrow{p} & R^d \\ \downarrow \sigma & & \downarrow s \\ V & \xrightarrow{p} & R^d \end{array} \tag{5}$$

As remarked above, it is convenient to keep p and π on an equal footing. Then (4) becomes the equivalent, but more revealing condition:

$$s \circ p = p \circ \sigma \quad \text{and} \quad C_s \circ \pi = \pi \circ C_\sigma \tag{6}$$

where C_s denotes the restriction to the group of translations $\mathcal{T}(R^d)$ of the conjugation by s in $E(d)$ and C_σ denotes the restriction to Γ of the conjugation by σ in $Aut(G)$.

With (p, π) given, it follows from (6) that s is uniquely determined by σ. Indeed, assuming the origin in R^d to be the image by p of a particular vertex $v_0 \in G$, we have:

$$s(x) = Sx + t, \tag{7}$$

$$\text{with } S = C_s \text{ when } R^d \equiv \mathcal{T}(R^d) \text{ and } t = s(0) = p(\sigma v_0) \tag{8}$$

Note that s is a translation if and only if C_s is the identity, that is, if and only if σ belongs to the centralizer $\mathcal{C}(\Gamma)$ of Γ in $N(\Gamma)$:

$$\mathcal{C}(\Gamma) = \{\delta \in N(\Gamma) \mid \delta\gamma = \gamma\delta \text{ for all } \gamma \in \Gamma\}$$

Thus, the set of all symmetries of (G, Γ, p, π) becomes a group under composition. This is the *symmetry group* of the framework and will be denoted by $\Sigma = \Sigma(G, \Gamma, p, \pi) \subset N(\Gamma) \subset Aut(G)$. The periodicity group Γ is a normal subgroup of Σ and the injective homomorphism $\sigma \mapsto s$ is an extension of $\pi : \Gamma \to \mathcal{T}(R^d)$ to $\Sigma \to E(d)$. For simplicity, this extension is also denoted by π. Since $\pi(\Sigma)$ is a crystallographic group, we may refer to the framework (G, Γ, p, π) as having *crystallographic symmetry* Σ.

2 Symmetry constraints

For a given $\sigma \in N(\Gamma)$, we may identify all periodic placements (p, π) for which σ is a symmetry of the framework (G, Γ, p, π). It will be convenient to give this description in terms of parameters based on the following *choices*: a complete set of representatives $v_0, v_1, ..., v_{n-1}$ for the vertex orbits of Γ on V and an isomorphism $Z^d \approx \Gamma$. Later on, a complete set of edge representatives of the form $e_{ij} = (v_i, v_j + \gamma_{ij})$ for the orbits of Γ on E will be implicated in obtaining equations for the length preservation of edges under deformation.

Note that we allow the additive notation $\gamma v = v + \gamma$ for the action of $\gamma \in \Gamma$ on a vertex of the graph, which will facilitate writing the corresponding translation in a placement (p, π) as $\pi(\gamma)p(v) = p(v) + \lambda$, when the translation $\pi(\gamma) \in \mathcal{T}(R^d)$ has the formula $\pi(\gamma)(x) = x + \lambda$ and is identified with the translation vector $\lambda \in R^d$.

Besides the frequent identification $\mathcal{T}(R^d) \equiv R^d$, which induces an inner product on the group of translations, other routine **conventions and notations** will be the following. With the chosen isomorphism $Z^d \approx \Gamma$, the automorphisms of the free Abelian group Γ are given by $d \times d$ matrices with integer entries and determinant ± 1, that is $Aut(\Gamma)$ is identified with the *unimodular group*

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$GL(d, Z)$. Moreover, by turning the free module Z^d into the d-dimensional vector space

$$R^d = Z^d \otimes_Z R \approx \Gamma \otimes_Z R$$

unimodular transformations will be conceived as linear transformations. In particular, conjugation by $\sigma \in N(\Gamma)$ gives an automorphism $C_\sigma \in Aut(\Gamma)$ and thereby a unimodular transformation which we denote by the same symbol $C_\sigma \in GL(d, Z)$. Thus, we have a representation $N(\Gamma) \to GL(d, Z)$ with kernel $\mathcal{C}(\Gamma)$.

When given a periodic placement (p, π) of (G, Γ), π gives an isomorphism

$$R^d \approx \Gamma \otimes_Z R \to \mathcal{T}(R^d) \equiv R^d \qquad (9)$$

Thus, two bases are at play: the fixed Cartesian standard basis of $R^d \equiv \mathcal{T}(R^d)$ and the *lattice basis* which depends on $\pi : Z^d \approx \Gamma \to \mathcal{T}(R^d)$. Sometimes, the coordinates based on the Cartesian basis are called *geometric* and those based on the periodicity lattice are called *arithmetic*.

We have seen above that a necessary condition for $\sigma \in N(\Gamma)$ to be a symmetry of the framework (G, Γ, p, π) is that $C_\sigma \in GL(d, Z)$ should be orthogonal, when expressed in Cartesian coordinates. The remaining conditions refer to the translation part t in (7), namely

$$t = p(\sigma(v_i)) - S(p(v_i)) \qquad (10)$$

which must be the same for all $i = 0, 1, ..., n-1$. It will be useful to express this in arithmetic coordinates. Let us assume that σ acts on the vertex representatives $v_0, v_1, ..., v_{n-1}$ according to the formulae:

$$\sigma(v_i) = v_{\sigma(i)} + \gamma_i \qquad (11)$$

where $\sigma(i)$ is the index corresponding to the permutation effect of σ on V/Γ and $\gamma_i \in \Gamma$. Recall that the arithmetic or lattice coordines are introduced through $\pi : \Gamma \to \mathcal{T}(R^d) \equiv R^d$ and the chosen identification $Z^d \approx \Gamma$. Note that the periods $\lambda_i \in \Gamma$ in (11) will correspond with $n_i \in Z^d$ and these vectors with integer entries depend only on σ and the lattice identification $Z^d \approx \Gamma$. We allow here the same symbol C_σ for the conjugation given by σ on Γ, its expression as an automorphism of Z^d and its extension to $Z^d \otimes_Z R$.

With e_k, $1 \le k \le d$ the standard basis in Z^d, we let $\Lambda_\pi = \Lambda \in GL(d, R)$ denote the matrix with columns given by the lattice basis $\pi(e_k)$. We define vector parameters t_i by

$$p(v_i) = \Lambda t_i \qquad (12)$$

and obtain from (10) and (11) the following conditions:

$$t_{\sigma(i)} + n_i - C_\sigma t_i = t_{\sigma(j)} + n_j - C_\sigma t_j, \quad \text{for} \ \ 0 \le i, j \le n-1 \qquad (13)$$

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Let us put $\omega_\pi = \omega = \Lambda^t\Lambda$ for the Gram matrix of the period lattice basis. Then, the orthogonality condition for $C_\sigma \in GL(d, Z)$ becomes:

$$C_\sigma^t \omega C_\sigma = \omega \tag{14}$$

In summary, we have

Proposition 2 *A graph automorphism $\sigma \in N(\Gamma) = Aut(G, \Gamma)$ is a symmetry of the d-periodic framework (G, Γ, p, π) if and only if conditions (13) and (14) are satisfied.*

Recall that the placement information (p, π) enters in these equations through the parameters t_i, $0 \leq i \leq n - 1$ and ω as described above. In subsequent sections, we shall elaborate on their role in describing symmetric periodic placements and symmetry preserving deformations.

3   Parametrizations

The deformation theory developed in [BS2] for periodic bar-and-joint frameworks in R^d emphasized the analogy with the traditional theory of finite linkages. In particular, equivalent realizations resulting from isometries applied to any given framework were not immediately factored out. However, enumerative purposes or other concerns require the quotient operation. In the finite case [BS1], Cayley-Menger matrices or equivalently, Gram matrices serve the purpose. In the periodic case, crystallography and lattice theory have proven long ago the importance of the identification of the quotient $O(d, R)\backslash GL(d, R)$ with the space of *positive definite quadratic forms* in d variables, itself represented by the open cone $\Omega(d)$ of symmetric $d \times d$ matrices with positive eigenvalues [CS, G, S1, W].

The parametrization used in the previous section follows this classical perspective. All the information about the lattice of periods $\pi(\Gamma)$, up to orthogonal transformations, is contained in the symmetric matrix $\omega = \Lambda^t\Lambda \in \Omega(d)$, while the 'shift vectors' t_i indicate (relative to the lattice basis) the placement of the vertex representatives v_i. By requesting that $t_0 = 0$, equivalence under translation is eliminated as well. This yields

Proposition 3 *Let (G, Γ) be a d-periodic graph. Then all periodic placements in R^d, up to equivalence under the group of Euclidean isometries $E(d)$, are parametrized by $(R^d)^{n-1} \times \Omega(d)$, which is an open set of $R^{dn+\binom{d}{2}}$.*

Remarks. The vertex image sets of periodic placements are multilattices and this type of configurations has been considered in different contexts. While not implicating an edge structure, the study of multilattices envisaged in [P, PZ] is related to the kinematics of phase transitions in crystalline materials. When

approached from the point of view of periodic sphere packings, as in [S1, S2], multilattices do acquire an edge structure from contacts between spheres. The resulting *packing frameworks* are a very particular class of periodic frameworks. A study of homogeneous sphere packings in dimension three has been undertaken by W. Fischer, E. Koch and H. Sowa in a series of papers e.g. [KSF]. The planar homogeneous case goes back to Niggli [N1, N2]. See also [F].

The bar-and-joint understanding of a framework brings in the (squared) length function for edges and the notion of deformations [BS2]. For a given d-periodic framework (G, Γ, p, π) vertices become joints and edges become straight rigid bars between them. It is enough to register the (squared) length of a complete set of representatives for E/Γ. As mentioned earlier, with vertex representatives $v_0, ..., v_{n-1}$ already chosen, we may select m edge representatives of the form $e_{ij} = (v_i, v_j + \gamma_{ij})$. For expressing the squared length in both geometric and arithmetic coordinates, we let $n_{ij} \in Z^d$ stand for the vector with Λn_{ij} equal to the translation vector of $\pi(\gamma_{ij})$. Then

$$\ell(e_{ij})^2 = ||p(v_j + \gamma_{ij}) - p(v_i)||^2 = (t_j + n_{ij} - t_i)^t \omega(t_j + n_{ij} - t_i) \qquad (15)$$

This gives a *polynomial map* with cubic $(i \neq j)$ or linear $(i = j)$ components.

$$f : (R^d)^{n-1} \times \Omega(d) \to R^m$$

$$f(t_1, ..., t_{n-1}, \omega) = ((t_j + n_{ij} - t_i)^t \omega(t_j + n_{ij} - t_i))_{ij} \in R^m$$

$$(16)$$

where the m pairs of indices ij correspond to the chosen representatives for the edge orbits E/Γ.

The non-empty fibers of this map are *configuration spaces of frameworks* and the connected component of a framework in its configuration space gives the *deformation space of the framework*.

For a simple comparison of this treatment with our presentation in [BS2], we offer the following diagram.

$$
\begin{array}{ccc}
(R^d)^n \times GL(d, R) & \xrightarrow{q} & E(d)\backslash(R^d)^n \times GL(d, R) \\
\downarrow & & \| \\
R^m & \xleftarrow{f} & (R^d)^{n-1} \times \Omega(d)
\end{array}
\qquad (17)
$$

$(R^d)^n \times GL(d, R)$ is the parametrization used in [BS2] for periodic placements which include all isometric replicas of all frameworks. Hence, the fibers of the left vertical arrow are *realization spaces* for weighted periodic graphs (G, Γ, ℓ), that is, periodic graphs with prescribed lengths for their edges. When isometries are factored out, we obtain, as stated above in Proposition 3, the parameter space $(R^d)^{n-1} \times \Omega(d)$ with the bottom map (16). With explicit formulae, we have the following description.

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$(R^d)^n \times GL(d, R)$ parametrizes periodic placements (p, π) by recording the positions of the n vertex representatives and the basis of the lattice of periods $\pi(\Gamma)$, that is, $(p(v_0), ..., p(v_{n-1}), \Lambda)$. The left action of the isometry group $E(d)$ on these parameters is given by

$$u(p(v_0), ..., p(v_{n-1}), \Lambda) = (u \circ p(v_0), ..., u \circ p(v_{n-1}), U\Lambda) \qquad (18)$$

for an isometry $u(x) = Ux + t$, with $U \in O(d, R)$ and $t \in R^d$. The *quotient map* q works by the formula

$$q(p(v_0), ..., p(v_{n-1}), \Lambda) = (t_1, ..., t_{n-1}, \omega) =$$
$$= (\Lambda^{-1}(p(v_1) - p(v_0)), ..., \Lambda^{-1}(p(v_{n-1}) - p(v_0)), \Lambda^t \Lambda) \qquad (19)$$

The left vertical arrow is the composition $f \circ q$.

A direct enumerative consequence of the current presentation will be an upper bound for the number of distinct possible configurations of a *minimally rigid periodic graph* with generic edge lenght prescriptions. Recall from [BS2, BS3] that minimally rigid periodic graphs have $m = dn + \binom{d}{2}$ edge orbits. In the generic case, the corresponding edge length constraints are independent. There can be no more than $\binom{d+1}{2}$ linear constraints $(i = j)$ among them, because all linear constraints affect only ω. Since the polynomial map (16) can be extented to *complex projective* coordinates in $P_m(C)$, we infer from Bézout's theorem the following bound.

Proposition 4 *Let (G, Γ) be a minimally rigid d-periodic graph with $n = |V/\Gamma|$ and $m = |E/\Gamma| = nd + \binom{d}{2}$. Let μ be the number of cubic edge constraints $(i \neq j)$ in (16). Then $dn - d \leq \mu \leq m$ and (G, Γ) has at most 3^μ non-congruent configurations in R^d for a generic prescription of edge lengths.*

Remark. This upper bound result is analogous to the one obtained in [BS1] for finite minimally rigid graphs.

4 Actions and representations

We may now return to symmetry considerations and elaborate on the *affine* nature of the symmetry constraints obtained in Proposition 2 in terms of placement parameters $(t_1, ..., t_{n-1}, \omega)$.

Let us recall that, by definition, $\sigma \in Aut(G, \Gamma)$ becomes a symmetry of a placement (p, π) when the effect of σ on the periodic graph (G, Γ) is *reproduced* by the effect of an isometry $s \in E(d)$ on the image of the graph determined by $p(V)$. In other words, the placements (p, π) and $(p \circ \sigma, \pi \circ C_\sigma)$ must be equivalent under the action of $E(d)$. Hence, in parameters $(t_1, ..., t_{n-1}, \omega)$, we must have one and the same point. By Proposition 2, the *fixed point locus* of such an action by σ is given by an *affine linear subvariety* and this fact leads to

the obvious expectation that the action itself is expressed by an affine map in the parameters $(t_1, ..., t_{n-1}, \omega)$.

This is indeed the case, as ensuing computations will confirm. In order to discuss the action of $Aut(G, \Gamma)$ on placements and the quotient parameter space $(R^d)^{n-1} \times \Omega(d) \subset R^{dn + \binom{d}{2}}$ as a *left action*, we adopt the following convention.

Definition 5 *Let $\sigma \in Aut(G, \Gamma)$ be an automorphism of a d-periodic graph (G, Γ). The left action of $Aut(G, \Gamma)$ on periodic placements in R^d is defined by the formula:*

$$\sigma(p, \pi) = (p \circ \sigma^{-1}, \pi \circ C_{\sigma^{-1}}) \tag{20}$$

Theorem 6 *When expressed in parameters $(t_1, ..., t_{n-1}, \omega)$, the action (20) corresponds with an affine representation*

$$A : Aut(G, \Gamma) \to Aff(dn + \binom{d}{2}) \tag{21}$$

which factors through $Aut(G, \Gamma)/\Gamma = Aut(G/\Gamma)$.

For any subgroup $\Gamma \subset \Sigma \subset Aut(G, \Gamma)$, the periodic placements of (G, Γ) with crystallographyc symmetry Σ are parametrized by the fixed locus of $A(\Sigma)$ in $(R^d)^{n-1} \times \Omega(d)$, that is

$$\mathcal{F}(\Sigma) = \{x \in (R^d)^{n-1} \times \Omega(d) \ : \ A(\sigma)x = x, \ \text{for all } \sigma \in \Sigma\} \tag{22}$$

The locus with full symmetry $\mathcal{F}(Aut(G, \Gamma))$ is not empty.

Proof: For the computation in coordinates $(t_1, ..., t_{n-1}, \omega)$, let us put

$$\sigma(t_1, ..., t_{n-1}, \omega) = (\tilde{t}_1, ..., \tilde{t}_{n-1}, \tilde{\omega})$$

and recall that $t_0 = \tilde{t}_0 = 0$. We have $\tilde{\omega} = \tilde{\Lambda}^t \tilde{\Lambda}$, with $\tilde{\Lambda} = \Lambda C_{\sigma^{-1}}$, hence

$$\tilde{\omega} = (C_{\sigma^{-1}})^t \omega C_{\sigma^{-1}} \tag{23}$$

Recall also that σ^{-1} induces a permutation on $\{0, ..., n-1\}$ by its effect on V/Γ. By (11) and (19), we find $\sigma^{-1}(v_j) = v_{\sigma^{-1}(j)} - C_{\sigma^{-1}}\gamma_{\sigma^{-1}(j)}$ and then

$$\tilde{t}_j = C_\sigma(t_{\sigma^{-1}(j)} - t_{\sigma^{-1}(0)}) + (n_{\sigma^{-1}(0)} - n_{\sigma^{-1}(j)}) \tag{24}$$

Formulae (23) and (24) give the explicit form of the action of σ, which is linear in the components of ω and affine in the components of t_j, $j = 1, ..., n-1$.

The resulting homomorphism (21) is obviously trivial on Γ. Since $Aut(G, \Gamma)/\Gamma = Aut(G/\Gamma)$ is finite, the image group must have at least one fixed point (the barycenter of an orbit).

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Corollary 7 *There is an inclusion reversing correspondence $\Sigma \mapsto \mathcal{F}(\Sigma)$ between subgroups $\Gamma \subset \Sigma \subset Aut(G,\Gamma)$ and a finite system of non-empty affine linear sections of $(R^d)^{n-1} \times \Omega(d)$ which parametrize periodic placements with a specified crystallographic symmetry.*

It may be observed that this approach obtains periodic placements for (G,Γ) with full symmetry $Aut(G,\Gamma)$ realized by corresponding crystallographic groups, *without recourse to a minimizing principle.* Other methods for proving the existence of placements with higher symmetry rely explicitly on some 'energy functional' minimization technique for finding 'barycentric placements' [DF] or a harmonic 'standard placement' [KS].

5   Relaxing or refining symmetry

Up to this point, our considerations have focused on a given d-periodic graph (G,Γ) with framework placements (G,Γ,p,π) in R^d. However, various problems may require a relaxation $\tilde{\Gamma} \subset \Gamma$ or a refinement $\Gamma \subset \hat{\Gamma}$ of the periodicity group. With the perspective gained in the preceding sections, we may introduce the following definition.

Definition 8 *Let $G = (V,E)$ be an infinite graph and let $\Gamma_1, \Gamma_2 \subset Aut(G)$ be free Abelian groups of rank d such that the corresponding d-periodic graphs (G,Γ_i) admit periodic presentations in R^d. Then, Γ_1 and Γ_2 are called commensurate when $\Gamma_1 \cap \Gamma_2$ is of finite index in both groups Γ_1 and Γ_2.*

Let us observe the effect of *relaxing* periodicity from Γ to a subgroup $\tilde{\Gamma} \subset \Gamma$ of index k. We select a complete set of representatives $\nu_0 = 0, \nu_1, ..., \nu_{k-1}$ for $\Gamma/\tilde{\Gamma}$. Then, representatives for $V/\tilde{\Gamma}$ are given by $v_i + \nu_j$, with $0 \leq i \leq n-1$ and $0 \leq j \leq k-1$.

When each periodicity group is identified with Z^d, the inclusion of $\tilde{\Gamma}$ in Γ corresponds to an invertible matrix with integer entries M with $det(M) = k$. Of course, the Γ-periodic placements of (G,Γ) are contained in the $\tilde{\Gamma}$-periodic placements of $(G,\tilde{\Gamma})$, and for a placement (p,π) this inclusion takes the form:

$$((t_i)_i, \omega) \mapsto ((\tilde{t}_{ij})_{ij}, \tilde{\omega}), \quad \text{with } t_0 = 0 = \tilde{t}_{00} \tag{25}$$

With $\pi(\nu_j) = m_j$ as translation vectors, we have $p(v_i + \nu_j) = p(v_i) + m_j$. By (19) and its counterpart for $\tilde{\Gamma}$, we find:

$$\tilde{\Lambda} = \Lambda M, \quad \text{hence } \tilde{\omega} = \tilde{\Lambda}^t \Lambda = M^t \omega M \tag{26}$$

$$\tilde{t}_{ij} = M^{-1} t_i + M^{-1} \Lambda^{-1} m_j \tag{27}$$

We already know that, from the perspective of $(G,\tilde{\Gamma})$, the placements with 'higher' symmetry Γ are parametrized by an affine linear section and the above

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computation confirms the expected fact that we have an affine inclusion map which identifies the parameter space for periodic placements of (G, Γ) with this affine linear section. It follows that *the affine and convexity structure* of the parameter space $(R^d)^{n-1} \times \Omega(d) \subset R^{dn+\binom{d}{2}}$ for periodic placements of (G, Γ) is preserved when relaxing the lattice.

Recall that a *crystallographic group* in dimension d is a *discrete* subgroup of isometries $K \subset E(d)$, with a *compact* quotient $E(d)/K$. Bieberbach showed that the subgroup of translations in K, that is $L = K \cap \mathcal{T}(R^d)$, must be a lattice of rank d and is uniquely determined as the maximal free Abelian normal subgroup of K. Moreover, K/L is a finite group. Thus, if $\Sigma \subset Aut(G)$ is isomorphic with a crystallographic group $K \subset E(d)$, we may refer to the free Abelian normal subgroup $\Gamma \subset \Sigma$ corresponding to $L \subset K$, and form the d-periodic graph (G, Γ).

We have seen above that, when (G, Γ) allows periodic placements in R^d, some of them, namely those parametrized by $\mathcal{F}(\Sigma)$, will have Euclidean symmetries given by some crystallographic group isomorphic with Σ and K (which must be, according to another Bieberbach theorem, an affine conjugate of K).

Under these circumstances, we may refer to $\Sigma \subset Aut(G)$ as a *crystallographic subgroup* of $Aut(G)$ and use the pair notation (G, Σ) for the graph G *with the specified crystallographic symmetry* Σ. It is also understood that, up to Euclidean isometry, the placements of (G, Σ) are those parametrized by $\mathcal{F}(\Sigma)$. We note that $\mathcal{F}(\Sigma)$ can be determined in the placement parameter space of any periodic graph $(G, \tilde{\Gamma})$ with $\tilde{\Gamma} \subset \Gamma$ of finite index and stable under conjugation by Σ. This determination amouts to solving a linear system of equations with integer coefficients of the form (13) and (14), corresponding to a finite set of transformations $\sigma \in \Sigma$ which provide generators for $\Sigma/\tilde{\Gamma}$. Verifications entirely similar to those performed above show that *the affine and convexity structure* of $\mathcal{F}(\Sigma)$ is the same for all choices of $\tilde{\Gamma}$.

The commensurability equivalence relation extends as follows.

Definition 9 *Two crystallographic subgroups $\Sigma_1, \Sigma_2 \subset Aut(G)$ are called commensurate when $\Sigma_1 \cap \Sigma_2$ is of finite index in both Σ_1 and Σ_2.*

Remarks. It would be enough to assume $\Sigma_1 \cap \Sigma_2$ of finite index in one of the groups, but we prefer the symmetric formulation. Clearly, in this case, the intersection $\Sigma_1 \cap \Sigma_2$ is itself a crystalographic subgroup of $Aut(G)$. Subgroups of finite index in crystallographic groups can be found by simple procedures [Se].

Relaxing or refining the symmetry of a framework are associated with certain variations within the framework's commensurability equivalence class. This language seems favorable for addressing geometric aspects of *displacive phase transitions* in crystalline materials [Bu, D]. The vertices of the infinite graph G may serve as labels for a subfamily or all of the atoms in some idealized crystal, with edges marking bonds. Under variations of temperature or pressure,

the same material may have phases with different crystallographic symmetry. Displacive phase transitions involve no bond rupture, hence the graph remains the same. When two phases have commensurate symmetry groups Σ_1, Σ_2, our approach gives the simplest geometrical common ground for a passage, namely $\mathcal{F}(\Sigma_1 \cap \Sigma_2)$, which contains both $\mathcal{F}(\Sigma_1)$ and $\mathcal{F}(\Sigma_2)$ as affine linear sections.

Of course, as a guiding scenario, this has been formulated long ago. The new insight, at least at the geometric level, is that the symmetry preserving loci have a simple affine structure and description. However, non-linearity resurfaces when bonds are assumed to maintain their length. This is considered in the next section.

6 Symmetry preserving deformations

When returning to the edge squared length function (16), a first simple remark is that f is $Aut(G, \Gamma)$ equivariant. To see this, it is convenient to write R^m as the space $R^{E/\Gamma}$ of real-valued functions on E/Γ. Then the left action of $Aut(G, \Gamma)$ is simply defined as

$$\sigma(\phi) = \phi \circ \sigma^{-1}, \quad \text{for } \phi \in R^{E/\Gamma} \tag{28}$$

with the action on E and on E/Γ denoted by the same symbol. Then, one easily verifies that

$$f(\sigma(p, \pi)) = \sigma(f(p, \pi)) \tag{29}$$

When given a framework (G, Γ, p, π) with crystallographic symmetry $\Sigma \subset N(\Gamma) = Aut(G, \Gamma)$, and we want to consider *only* deformations which preserve this symmetry (and all edge lengths), we have to restrict f to $\mathcal{F}(\Sigma)$ and consider the fiber of $f(p, \pi)$. Since Σ acts trivially on $\mathcal{F}(\Sigma)$, the image by f must consist of points invariant under Σ, that is, f factors through $R^{E/\Sigma}$.

Remark. Strictly speaking, we should write $\Sigma \backslash E$ for the quotient by an action on the left. Expecting no harm, we continue with E/Σ and note that $E/\Gamma \to E/\Sigma$ induces $R^{E/\Sigma} \to R^{E/\Gamma}$.

It follows that the edge length control for frameworks with crystallographic symmetry Σ is given by a map which we allow to be denoted by the same symbol

$$f : \mathcal{F}(\Sigma) \to R^{E/\Sigma} \tag{30}$$

Thus, after appropriate rank computations, we obtain a setting entirely analogous to the basic case $\Sigma = \Gamma$.

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